In The Name of GOD

Contents

User's Guide for Grating and Photonic Crystal Package

1. Introduction

This package is a collection of MATLAB programs for the analysis of diffraction gratings and 2D photonic crystals. Indeed, every 2D structure which is periodic in one of its dimensions and arbitrary shaped in the other dimension can be analyzed by this package. The LPEM (Legendre polynomial expansion method) is employed here [1]. Although it is not necessary for users to be familiar with this method, I recommend reading Ref.1 for better understanding of the codes.

In this document you learn how to define and analyze an arbitrary structure with this package. You are also guided to use proper m-files for some conventional structures like square lattice and triangular lattice photonic crystals, lamellar gratings, trapezoidal and sinusoidal surface relief gratings and volume gratings.

2. Calculating the R matrix of a periodic layer

A typical periodic layer, as shown in Fig.1, is infinite and periodic in one direction (x) and finite with arbitrary permittivity profile in the other direction (z). In other words, the permittivity function can be written as,

$$\varepsilon(x + \Lambda_G, z) = \varepsilon(x, z), \quad 0 < z < d, \quad -\infty < x < \infty. \tag{1}$$

where Λ_G and d (denoted by `d` in the code) are the grating period and thickness, respectively. Hereafter, we assume that all lengths are normalized to the grating period so we put $\Lambda_G = 1$.
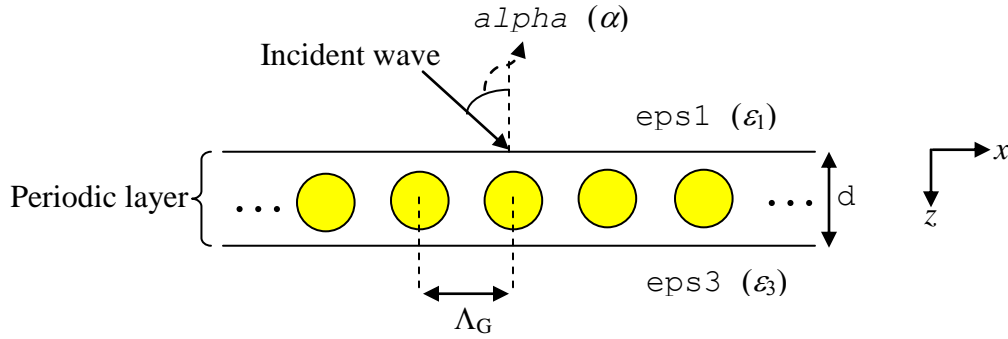
Figure 1. Schematic of a periodic layer (grating layer)

The upper and the lower regions called incident and transmission mediums, respectively, are homogenous. Their permittivity are denoted `eps1` (ε_1) and `eps3` (ε_3) through the m-file.

The incident wave is a TE (electric field in y direction) or TM (magnetic field in y direction) polarized plane wave. Its wavelength (λ) and incident angle (α) are determined with variables `lambda` and `alpha`, respectively.

A. Defining a periodic layer

To define a periodic layer we use two matrices `xt` and `epst` which their columns determine discontinuity places and the permittivity between discontinuities for each z, respectively. Let us see how we can fill these two matrices through two examples.

The first example is an array of circles (rods) as shown in Fig. 1. One period of this layer is illustrated in Fig. 2. Before specifying `xt` and `epst` we have to define the vector `z` that determines z coordinate's points. Since the Gauss-Legendre algorithm is used in this package for integration, the spacing between elements of `z` is not uniform and you should use following instructions to produce `z`:

```
n = L * nlayer;
z = LPEM_zgen15(d,n);
```

where d is the periodic layer (the grating) thickness and L and nlayer are two convergence parameters (see the next part: Adjusting convergence parameters) and they are previously determined. The length of z will be 15 * n.
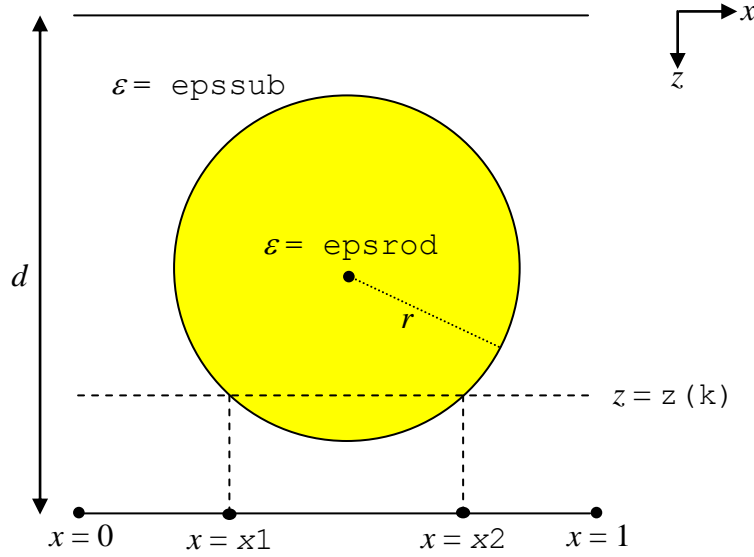
Figure 2. One period of a grating layer consist of an array of circular rods.

Now we should determine xt and epst at each z. For instance, assume that $z = $ z(k) and discontinuities are at x = x1, x2 as depicted in Fig. 2. Then we have,

```
xt(1,k)  = x1;
xt(2,k)  = x2;

epst(1,k)  = epssub;
epst(2,k)  = epsrod;
epst(3,k)  = epssub;
```

The first two lines mean that at $z = $ z(k) the first discontinuity is at x1 and the second one is at x2. The last three lines mean that in intervals (0, x1), (x1, x2) and (x2, 1) the permittivities are epssub, epsrod and epssub, respectively. For values of z that no discontinuity exist we can put x1 = x2 = 0.5.

An important point is that the number of rows of epst is equal to that of xt plus 1.

In summary, following command lines can lead to the structure in Fig. 2:

```
z=LPEM_zgen15(d,n);
zlen =  length(z);

xt=zeros(2,zlen);
epst = zeros(3,zlen);

epst(1,:)= epssub;
epst(2,:)  = epsrod;
epst(3,:)  = epssub;

xt(1,:)=.5;
xt(2,:)=.5;

for k=1:zlen
    if (z(k)>d/2-r)&&(z(k)<d/2+r)
        xt(1,k)=1/2-sqrt(r^2-(z(k)-d/2)^2);
        xt(2,k)=1/2+sqrt(r^2-(z(k)-d/2)^2);
    end
end
```
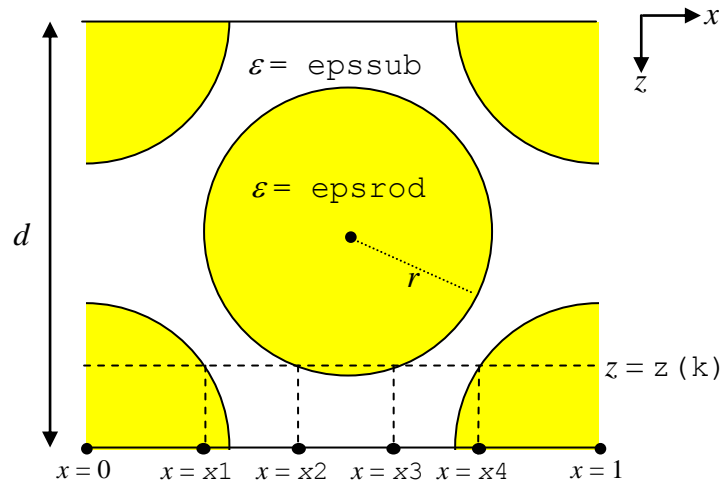
To verify that the structure has been correctly defined, you can use following command,

```
plot(xt(1,:),z,xt(2,:),z)
```


Figure 3

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One period of the second structure, which is more complicated than the previous one, is shown in Fig. 3. In this case for some values of z there are four discontinuities, as a result the number of rows of `xt` should be 4 and that of `epst` should be 5. In accordance to Fig. 3, at $z = $ `z(k)` we have

```
epst(1,k) = epsrod;
epst(2,k) = epssub;
epst(3,k) = epsrod;
epst(4,k) = epssub;
epst(5,k) = epsrod;

xt(1,k) = x1;
xt(2,k) = x2;
xt(3,k) = x3;
xt(4,k) = x4;
```

See "TriangularLatticeCircularRod15.m" for finding out in detail how to produce this structure.

B. Adjusting convergence parameters

You should be sure that the obtained result has been converged to the accurate one. On the other hand, the simulation time should not be too long. To achieve a compromise between these two factors (i.e. the accuracy and the simulation time), four variables called convergence parameters have to be carefully adjusted. These variables are `N`, `L`, `M` and `nlayer`, corresponding to truncation order, number of layers, number of polynomial terms and integration accuracy parameter, respectively. For complete understanding of these parameters one should read [1], but for using the codes the concise information given here is enough.

Recommended values for `M` and `nlayer` are 3 and 1 in TM polarization and, 6 and 5 in TE polarization. So you should only adjust `N` and `L` in order to reach to an accurate result. First you should increase `L` and verify the result not to change very much and then increase `N`. It is very difficult to say exactly which values are proper for `N` and `L`, because it depends on wavelength, the grating thickness, the permittivity contrast and even polarization. However if you choose $5 < $ `N` $ < 20$ and 10`d` $< $ `L` $ < 100$`d`, you will usually obtain proper accuracy and simulation time for many structures in optical frequencies. Nevertheless, you should be very careful of high contrast permittivity profiles, especially deep ones, which may need large truncation order and layer numbers even larger than the above suggested values.

If you don't see `L` and `nlayer` as convergence parameters in some codes, you shall set `M` = 3 and change other parameters to achieve the convergent result. This happens when you want to use m-files related to volume and lamellar gratings.

C. Using RmatrixTE.m and RmatrixTM.m

Now we are at a point that the R matrix of the structure can be easily computed. This can be achieved by using the functions RmatrixTE.m and RmatrixTM.m which are for TE and TM polarization, respectively. One should only type following command, after setting necessary variables described in preceding parts,

```
[R11 R12 R21 R22] = RmatrixTE(xt,epst,d,lambda,alpha,eps1,N,M,L,nlayer)
```

or

```
[R11 R12 R21 R22] = RmatrixTM(xt,epst,d,lambda,alpha,eps1,N,M,L,nlayer)
```

for TE and TM polarization, respectively. The R matrix of the grating layer will be,

```
R = [R11 R12
     R21 R22];
```

D. Multilayer structures and R matrix algorithm

In many problems you may encounter multilayer gratings. For example, a slice of photonic crystal is a repetition of a periodic layer.

Given the R matrix of different layers, you can obtain the overall R matrix with the R matrix algorithm [1],[2].
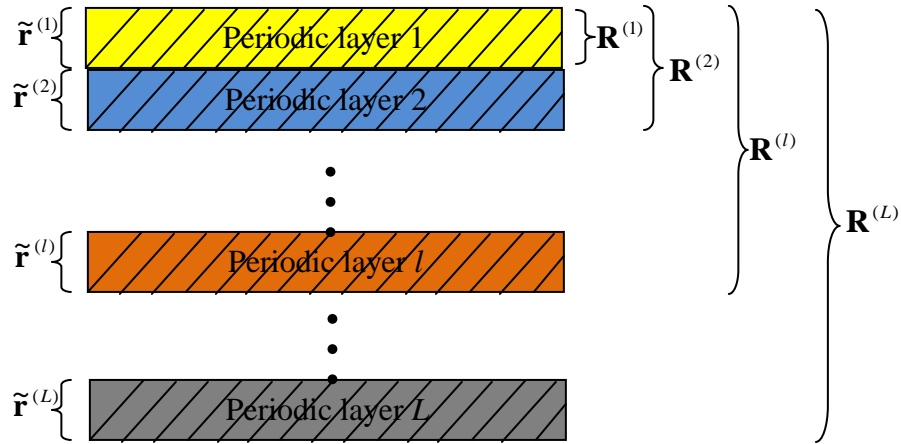

Figure 4. Schematic of a multilayer grating.

Let's denote the R matrix of lth layer with $\tilde{\mathbf{r}}^{(l)}$ and the total R matrix from layer 1 to layer l with $\mathbf{R}^{(l)}$ (see Fig. 4). Now, the overall R matrix of L layers, $\mathbf{R}^{(L)}$, can be calculated by the following recursion formula:

$$\mathbf{R}_{11}^{(l)} = \tilde{\mathbf{r}}_{11}^{(l)} - \tilde{\mathbf{r}}_{12}^{(l)} \mathbf{Z}^{(l)} \tilde{\mathbf{r}}_{21}^{(l)},$$

$$\mathbf{R}_{12}^{(l)} = \tilde{\mathbf{r}}_{12}^{(l)} \mathbf{Z}^{(l)} \mathbf{R}_{12}^{(l-1)},$$

$$\mathbf{R}_{21}^{(l)} = -\mathbf{R}_{21}^{(l-1)} \mathbf{Z}^{(l)} \tilde{\mathbf{r}}_{21}^{(l)},$$

$$\mathbf{R}_{22}^{(l)} = \mathbf{R}_{22}^{(l-1)} + \mathbf{R}_{21}^{(l-1)} \mathbf{Z}^{(l)} \mathbf{R}_{12}^{(l-1)}, \tag{2}$$

where

$$\mathbf{Z}^{(l)} = (\tilde{\mathbf{r}}_{22}^{(l)} - \mathbf{R}_{11}^{(l-1)})^{-1} \tag{3}$$

and the recursion process is initialized by setting $\mathbf{R}^{(1)} = \tilde{\mathbf{r}}^{(1)}$.

3. Computing diffraction efficiencies

Diffraction efficiency is the proportion of the active power carried by each diffracted order to the power of incident wave. This parameter can be easily computed in this package. To this end type

```
[R11 R12 R21 R22] = RmatrixTE(xt,epst,d,lambda,alpha,eps1,N,M,L,nlayer)
[DE1 DE3] = DETE(R11,R12,R21,R22,lambda,alpha,eps1,eps3)
```

for TE polarization. In TM polarization case, replace `TE` with `TM`.

`DE1(j)` and `DE3(j)` are the diffraction efficiencies of the $N + 1 - j$ reflected and transmitted orders, respectively.

4. Band structure computation for photonic crystals

Having known the R matrix of one layer of a photonic crystal, the band structure can be easily calculated [3]. The R matrix of a layer is a function of wavelength (or frequency) and propagation constant of incident wave in x direction. The latter is exactly the x component of Bloch wave number κ, in other words, $\kappa_x = \dfrac{2\pi}{\lambda} \sqrt{\varepsilon_1} \sin\alpha$ (`kappax = 2 * pi * (eps1 ^ 0.5) * sin(alpha) / lambda`). Consequently, the z component is only needed. You can easily calculate this parameter using this command,

```
kappaz = Blochwavenumber(R11,R12,R21,R22,d)
```

5. Other functions and codes

In this section we give the list of other functions and codes available in this package and briefly describe their application.

Function or code	Application
FP_TE.m FP_TM.m	These functions are for computing the field profile and the diffraction efficiencies of a grating with discontinuous permittivity profile.
LPEM_TE_Lamellar.m, LPEM_TE_Lamellar_FP.m, LPEM_TM_Lamellar.m, LPEM_TM_Lamellar_FP.m	These codes are for the efficient analysis of multilayer lamellar gratings. The codes with FP suffix are for field profile calculation.
LPEM_TE_PhC.m, LPEM_TE_PhC_FP.m, LPEM_TM_PhC.m, LPEM_TM_PhC_FP.m	These codes are for the analysis of typical photonic crystals: square and triangular lattice with circular rods. The codes with FP suffix are for field profile calculation.
LPEM_TE_SurfaceRelief.m, LPEM_TM_SurfaceRelief.m	These codes are for the analysis of typical surface relief gratings: sinusoidal, trapezoidal and triangular surfaces.
LPEM_TE_Volume.m, LPEM_TM_Volume.m	These codes are for the analysis of longitudinally homogenous and inhomogenous volume gratings.
RmatrixTE_hom.m, RmatrixTM_hom.m	These functions are for efficient calculation of the R matrix of a homogenous layer.
RmatrixTE_vol.m, RmatrixTM_vol.m	These functions are for efficient calculation of the R matrix of a longitudinally homogenous volume grating.
RmatrixTE_lam.m, RmatrixTM_lam.m	These functions are for efficient calculation of the R matrix of a longitudinally homogenous lamellar grating.

References

[1] A. Khavasi, A. K. Jahromi, and K. Mehrany, "Longitudinal Legendre polynomial expansion of electromagnetic fields for analysis of arbitrary-shaped gratings," J. Opt. Soc. Am. A, **24**, 1564-1573 (2008).

[2] L. Li, "Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings," J. Opt. Soc. Am. A. **13**, 1024-1035 (1996).

[3] B. Gralak, S. Enoch, and G. Tayeb, "Anomalous Refractive Properties of Photonic Crystals," J. Opt. Soc. Am. A **17**, 1012-1020 (2000).